Indian J. Phys. **79(4)**, 409-415 (2005)

Note

AN INTERNATIONAL JOURNAL

IJP

Franck Condon factors and *r*-centroids of the *A*-*X* and *B*-*X* band systems of GaCl and GaI molecules

M D Saksena* and Sunanda K

Spectroscopy Division, Modular Laboratories, Bhabha Atomic Research Centre, Trombay, Mumbai-400 085, India

E-mail : sunanda@magnum.barc.ernet.in

Received 23 June 2004, accepted 31 January 2005

Abstract : High resolution studies of the electronic spectra of GaCl and GaI carried out in our laboratory, have led to accurate rotational and vibrational constants of the excited states. Using these constants, the Franck Condon factors and *r*-centroids were computed for the bands of the $A^1\Pi_0 - X^1\Sigma^+$ and $B^3\Pi_1 - X^1\Sigma^+$ transitions in these molecules. Comparisons of the visually estimated intensities of the observed bands recorded on a 3.4 m Ebert grating spectrograph showed reasonable agreement with the computed Franck Condon factors. These results indirectly ascertained the vibrational numbering of the vibrational band heads after head of heads formation in GaCl and reversal of the degradation in GaI.

Keywords : Franck Condon factors, *r*-centroids, electronic transitions, GaCl and GaI molecules

PACS Nos. : 33.70.Ca, 33.20.Lg

The electronic spectra of gallium chloride (GaCl) and gallium iodide (GaI) have been studied in absorption as well as in emission, mostly confining to the ground and low-lying excited states [1–4 and references therein]. The electronic spectra of the homologous group of molecules belonging to the 10 valence electrons, formed from atoms of group IIIA and group VIIA molecules, comprise of three prominent band systems *viz.* $A^3\Pi_0 - X^1\Sigma^+$ and $B^3\Pi_1 - X^1\Sigma^+$ and $C^1\Pi - X^1\Sigma^+$ transitions. The overlapping bands of *A*-*X* and *B*-*X* in GaCl are observed in the 320–350 nm spectral region while the *C*-*X* system is observed between 240–270 nm. In GaI, the overlapping *A*-*X* and *B*-*X* band systems appear in the 380–420 nm region while a continuous absorption with a maximum at 306.5 nm was attributed to the *C*-*X* transition. In the recent past, we have carried out detailed vibrational and rotational analyses using single enriched isotopes of gallium (^{69}Ga/^{71}Ga). For confirmation of the vibrational assignments of large number of new bands of both GaCl and GaI, isotopic shift studies have also been done. The spectra of *A*-*X* and *B*-*X* transitions in these molecules were recorded using the two stable isotopes of gallium *viz.* ^{69}Ga (60%) and ^{71}Ga (40%). The use of single isotope of gallium not only helped in confirming many of the vibrational assignments, but also simplified the rotational structure. The ground state $X^1\Sigma^+$ in these molecules has been well studied through microwave studies [5,6]. The Franck Condon factors (FCF) and *r*-centroids (RC) for the bands of *A*-*X* and *B*-*X* systems of these molecules are computed using our constants which shed light on the intensity distribution among these bands.

The emission spectra of ^{69}GaCl/^{71}GaCl and ^{69}GaI/^{71}GaI are excited in similar experimental conditions using a sealed quartz electrodeless discharge lamp, employing microwaves (245 MHz, 150 W). Details of the experimental procedure are given in our earlier papers [1,3].

The Franck Condon principle, assuming that the electronic transition moment does not vary over the band system, can largely explain the intensity distribution in the band system. The molecular constants for the upper states from our earlier work [1–4] along with the ground state microwave coefficients [5,6], have been used to evaluate the Franck Condon factors (FCF's) and *r*-centroids of the systems using TRAPRB programme developed by Jarmain and McCallum [7]. In this program,

*Corresponding Author

the Klein-Dunham series is used to represent the spectroscopic input data, namely, the vibrational and rotational constants. The RKR potential curves are then computed. The Schrödinger wave equation is solved numerically and the resulting vibronic eigenfunctions are used to calculate the Franck Condon factors and r-centroids. Table 1 lists the molecular constants used in calculating the FCF's and r-centroids.

Table 1. Constants used in the evaluation of Franck Condon factors and r-centroids (cm^{-1})

State	$X^1\Sigma^+$	$A^3\Pi_0$	$B^3\Pi_1$
	$^{69}Ga^{35}Cl$ [Refs. 1,2]		
ω_e	365.32	395.13	394.71
$\omega_e x_e$	1.221	2.278	2.286
$\omega_e y_e$	–	–0.0177	–0.0205
B_e	0.1499031	0.158484	0.158107
α_e	0.0007899	0.00105	0.001050
$D_e \times 10^{-7}$	1.004	1.041	1.046
	$^{71}Ga^{127}I$ [Refs. 3,4]		
ω_e	214.64	190.67	183.49
$\omega_e x_e$	0.46	1.51	2.68
$\omega_e y_e$	–	–0.08	–
B_e	0.0558935	0.057947	0.057129
α_e	0.000179	0.000456	0.00045
$D_e \times 10^{-7}$	0.1517	0.2062	0.2255
$\beta_e \times 10^{-8}$	0.006	0.146	
$H_e \times 10^{-15}$	–0.456		

The FCF's and r-centroids calculated for the bands of the A-X and B-X systems of GaCl are given in Tables 2a and 2b, respectively. In the spectra of GaCl, the formation of head of heads was observed in the $\Delta v \geq +1$ sequences. The bands that appear after these head of heads formation, are found to have comparable Franck Condon factor values, which could indirectly confirm their vibrational assignments. The motivation to take up studies of GaCl spectra [1,2] was to consider the possibility of extending the vibrational scheme of A-X and B-X band systems to include the large number of red-degraded bands that were consistently observed in our experiments. It was thought that most likely these could be higher members of $\Delta v \geq +1$ sequences. Before the head of heads formation, in both A-X and B-X band systems, the bands are violet degraded. In the absence of band origin data, the head positions of these violet degraded bands have been used to obtain the vibrational coefficients. It is difficult to assign the red-degraded bands, as at higher v's, it may be necessary to include higher order vibrational coefficients and also because of the change of degradation, after a gap of number of bands, the extrapolation results in inaccurate band positions. However, the FCF's presented in Tables 2a and 2b, show that the higher members of $\Delta v \geq +1$ band systems have sufficient intensity even after the head of heads formation (Table 1 of Ref. [1]).

The FCF's values for the bands of the A-X and B-X transitions in GaI are listed in Tables 3a and 3b, respectively. The spectrum of GaI showed some bands with violet degradation and some with intensity patch. Also on the higher wavelength side, there appeared a group of red degraded bands. These bands were vibrationally assigned to belong to the higher members of negative sequences of the GaI A-X and B-X systems (Tables 1 and 2 in Ref. [3]). Calculations of the FCF's and r-centroids for these band systems in the present study, helped greatly in confirming our vibrational numbering. The low Franck Condon factor values for the initial members of $\Delta v \geq +2$ sequences explain the absence of these bands in the vibrational analysis. Another noticeable observation in the spectrum of the A-X band system was that the $\Delta v = -3$ sequence is weakest in comparison to those of $\Delta v = 1, 0, -1, -2$ and -4 which is confirmed by the low values of FCF's for these sequences. Also for $\Delta v = -5$ to -13 sequences, the initial members are absent, but a few higher members are observed. Comparison of the observed band intensities to the intensities calculated through the FCF's, made it possible to corroborate the vibrational assignments of the bands in the electronic transitions that are rather extensive. The agreement of intensities with the FCF's is only qualitative, as the potential used in the calculation (Hulburt-Hirschfelder function) may not be truly representative (especially for the high v values).

The electronic spectral studies of GaCl and GaI showed interesting features like head of heads formations and reversal of the degradation of the bands and a large number of extra bands. The purpose of this study was not to use an exact potential for calculation of FCF's and r-centroids but to grossly know whether the extra bands observed in both GaCl and GaI molecules could be included in the vibrational schemes of A-X and B-X band systems or not. The refined rotational and vibrational constants in the $A^3\Pi_0$, $B^3\Pi_1$ and $X^1\Sigma^+$ states of GaCl and GaI (Table 1) were used in obtaining the FCF's and r-centroids for the bands of A-X and B-X systems. These values qualitatively helped us in confirming the vibrational assignments by comparing the visually estimated intensities and also in confirming that in GaCl, the bands even after the change of degradation indeed belong to the A-X and B-X band systems. In the case of GaI, it was confirmed

v′/v″	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
0	**0.6285**	**0.2761**	**0.0755**	**0.0163**	0.0030																
	2.1753	2.1129	2.0590	2.0093	1.9621																
1	**0.3098**	**0.1880**	**0.3000**	**0.1440**	**0.0446**	0.0108	0.0023														
	2.2425	2.1884	2.1191	2.0641	2.0142	1.9671	1.9218														
2	**0.0570**	**0.3927**	0.0292	**0.2332**	**0.1813**	**0.0759**	0.0232	0.0058	0.0013												
	2.3210	2.2514	2.2196	2.1256	2.0691	2.0189	1.9719	1.9270	1.8836												
3	**0.0046**	**0.1284**	**0.3715**	0.0003	**0.1506**	**0.1879**	**0.1031**	0.0385	0 0114	0.0029											
	2.4243	2.3299	2.2611	1.7687	2.1327	2.0740	2.0234	1.9765	1.9319	1.8891											
4		**0.0142**	**0.1949**	**0.3109**	0.0225	**0.0822**	**0.1724**	**0.1220**	0.0546	0.0188	0.0054	0.0014									
		2.4358	2.3391	2.2720	2.1374	2.1414	2.0789	2.0277	1.9809	1.9365	1.8942	1.8544									
5			**0.0279**	**0.2495**	**0.2429**	0.0573	**0.0360**	**0.1448**	**0.1313**	0.0697	0.0275	0.0090	0.0026								
			2.4476	2.3485	2.2846	2.1596	2.1537	2 0838	2.0318	1.9850	1 9409	1.8992	1.8600								
6				0.0441	**0.2915**	**0.1816**	0.0881	0.0104	0.1129	**0.1316**	0.0822	0.0369	0.0135	0.0043	0.0013						
				2.4597	2.3581	2.2998	2.1689	2.1783	2.0888	2 0357	1.9889	1.9451	1.9038	1.8653	1.8308						
7				0.0016	**0.0614**	**0.3224**	**0.1320**	0.1091	0.0006	0.0821	0.1248	0.0911	0.0462	0.0188	0.0066	0.0022					
				2.6982	2.4723	2.3681	2 3187	2.1741	2.3148	2.0942	2.0394	1.9925	1.9490	1.9082	1.8703	1.8365					
8					0.0022	**0.0785**	**0.3452**	**0.0945**	0.1200	0.0015	0 0555	0.1128	0.0960	0.0547	0.0246	0.0095	0.0034	0.0011			
					2.7412	2.4852	2.3784	2.3428	2.1867	2.0229	2.1004	2.0430	1.9959	1.9527	1.9124	1.8751	1.8414	1.8145			
9						0.0027	0.0946	0 3623	**0.0674**	0.1222	0.0086	0.0343	**0.0978**	**0.0971**	**0.0619**	**0.0305**	**0.0129**	**0.0049**	**0.0018**		
						2.7953	2.4988	2.3892	2 3740	2 1772	2.0946	2.1085	2.0465	1.9992	1.9561	1.9163	1.8795	1 8469	1 8199		
10							0.0028	0.1090	0.3764	0.0487	0.1180	0.0186	0.0189	0.0815	0.0947	0 0672	0.0364	0.0166	0.0068	0 0027	0.0010
							2 8671	2.5129	2.4003	2.4141	2.1753	2.1140	2.1203	2.0499	2.0022	1.9593	1.9199	1.8837	1.8516	1.8250	1.8005
11								0.0025	0.1211	0.3892	0.0364	0.1095	0.0293	0.0087	0.0655	0.0894	0.0705	0.0416	0.0205	0.0091	0.0038
								2 9705	2.5278	2.4118	2.4644	2.1704	2.1246	2.1413	2.0533	2 0051	1 9623	1.9233	1.8876	1.8560	1.8298
12										0.1302	0.4025	0.0291	0.0983	0.0393	0.0028	0.0507	0.0820	0.0717	0.0459	0.0243	0.0115
										2.5437	2.4237	2.5238	2.1616	2.1326	2.1917	2.0569	2 0080	1.9651	1.9264	1.8912	1.8601
13											0.1355	0.4174	0.0256	0.0860	0.0481	0.0003	0.0380	0.0735	0.0710	0.0490	0.0278
											2.5611	2.4359	2.5868	2.1474	2.1400	2.4369	2.0605	2.0108	1.9676	1 9293	1.8945
14												0.1359	0.4348	0.0255	0.0733	0.0551	0.0001	0.0277	0.0647	0.0685	0.0507
												2.5806	2.4485	2.6439	2.1252	2.1483	1.5190	2.0642	2.0137	1.9699	1.9319
15													0.1302	0.4548	0.0293	0.0609	0.0606	0.0001	0.0200	0.0564	0.0649
													2.6034	2.4614	2.6846	2.0912	2.1587	1.8562	2.0673	2.0167	1.9719
16												0.0038	0.0014	0.1171	0.4766	0.0380	0.0492	0.0649	0.0021	0.0145	0 0493
												2.4785	1.3308	2.6317	2.4745	2.7036	2.0387	2.1726	1.8917	2.0683	2.0202
17													0.0050	0.0054	0.0958	0.4970	0.0540	0.0381	0.0686	0.0026	0.0110
													2.5385	1.9182	2.6696	2.4877	2.7035	1.9560	2.1917	1.8713	2.0640
18														0.0056	0.0134	0.0675	0.5105	0.0802	0.0275	0.0723	0.0023
														2.6063	2.1539	2.7261	2.5011	2.6913	1.8199	2.2180	1.8003

Table 2b. Franck Condon factors and r-centroids for the $B^3\Pi_0 - X^1\Sigma^+$ transition of $^{69}Ga^{35}Cl$.

v'/v''	0	1	2	3	4	5	6	7	8	9	10
0	**0.6536**	**0.2638**	**0.0666**	**0.0133**	0.0023						
	2.1766	2.1113	2.0551	2.0030	1.9530						
1	**0.2940**	**0.2243**	**0.3025**	**0.1316**	**0.0373**	**0.0084**	0.0016				
	2.2468	2.1891	2.1174	2.0602	2.0079	1.9582	1.9097				
2	**0.0489**	**0.3885**	0.0499	**0.2514**	**0.1723**	**0.0654**	**0.0183**	0.0042			
	2.3290	2.2557	2.2134	2.1236	2.0652	5.0126	1.9630	1.9147			
3	**0.0035**	**0.1123**	**0.3853**	0.0015	**0.1775**	**0.1863**	**0.0916**	**0.0311**	0.0084	0.0020	
	2.4393	2.3383	2.2654	2.3908	2.1301	2.0699	2.0171	1.9673	1.9183	1.8746	
4		**0.0108**	**0.1739**	**0.3406**	0.0089	**0.1099**	**0.1795**	**0.1119**	**0.0454**	0.0143	0.0038
		2.4518	2.3477	2.2760	2.0991	2.1374	2.0745	2.0208	1.9701	1.9253	1.8802
5			**0.0213**	**0.2270**	**0.2835**	0.0356	0.0590	0.1595	**0.1248**	**0.0596**	0.0214
			2.4648	2.3574	2.2880	2.1456	2.1461	2.0785	2.0232	1.9764	1.9298
6				**0.0336**	**0.2703**	**0.2283**	0.0640	0.0259	0.1333	**0.1306**	**0.0728**
				2.4782	2.3673	2.3018	2.1590	2.1576	2.0811	2.0292	2.9802
7					**0.0468**	**0.3048**	**0.1809**	0.0866	0.0077	0.1066	0.1316
					2.4922	2.3774	2.3177	2.1641	2.1732	2.0883	2.0326
8					0.0011	**0.0596**	**0.3323**	**0.1431**	0.1014	0.0007	0.0840
					2.8422	2.5067	2.3875	2.3349	2.1633	2.3171	2.0931
9						0.0012	0.0714	0.3547	**0.1147**	0.1087	0.0005
						2.9288	2.5211	3.3964	2.3493	2.1673	2.0137
10							0.0011	0.0813	0.3734	0.0953	0.1102
							3.0306	2.5338	2.4018	2.3887	2.1638

Table 3a. Franck Condon factors and r-centroids for the $A^2\Pi_0 - X\ ^2\Sigma^+$ transition of GaCl.

V'/V''	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0	**0.7762**	**0.1691**	**0.0433**	**0.0091**	0.0019											
	2.5580	2.4646	2.4337	2.3884	2.3567											
1	**0.2178**	**0.4773**	**0.1940**	**0.0815**	**0.0220**	**0.0057**	0.0013									
	2.6408	2.5733	2.4520	2.4337	2.3824	2.3544	2.3172									
2	0.0051	**0.3417**	**0.3305**	**0.1670**	**0.1070**	**0.0341**	**0.0109**	0.0028								
	2.9024	2.6488	2.5959	2.4317	2.4360	2.3742	2.3528	2.3119								
3		0.0079	**0.4151**	**0.2624**	**0.1244**	**0.1233**	**0.0426**	**0.0167**	0.0048	0.0014						
		2.9732	2.6580	2.6245	2.3984	2.4421	2.3622	2.3530	2.3048	2.2828						
4		**0.0037**	0.0060	**0.4558**	**0.2377**	**0.0808**	**0.1360**	0.0464	**0.0229**	0.0069	0.0025					
		2.5326	3.1121	2.6678	2.6554	2.3417	2.4536	2.3441	2.3562	2.2947	2.2828					
5			**0.0104**	0.0015	**0.4672**	**0.2380**	**0.0430**	**0.1498**	0.0449	**0.0299**	0.0089	0.0039	0.0013			
			2.5835	3.5373	2.6779	2.6843	2.2398	2.4718	2.3158	2.3645	2.2793	2.2862	2.2293			
6				**0.0218**	0.0008	**0.4456**	**0.2505**	**0.0154**	**0.1689**	0.0381	**0.0385**	0.0104	0.0060	0.0019		
				2.6277	3.8793	2.6877	2.7084	2.0363	2.4973	2.2696	2.3804	2.2543	2.2955	2.2142		
7					**0.0363**	0.0144	**0.3864**	**0.2617**	**0.0015**	**0.1961**	**0.0270**	**0.0505**	0 0106	0.0092	0.0027	0 0018
					2.6689	2.0495	2.6966	2.7266	1.5282	2.5291	2.1912	2.4065	2.2119	2 3144	2.1882	2.2414
8						0.0492	0.0540	**0.2917**	**0.2553**	**0.0019**	**0.2312**	**0.0140**	**0.0683**	**0.0091**	0.0144	0 0032
						2.7105	2.3925	2.7036	2.7338		2.5649	2.0486	2.4443	2.1363	2.3472	2.1409
9						0.0048	0.0522	0.1248	**0.1772**	**0.2168**	**0.0117**	**0.2687**	**0.0034**	**0.0951**	**0.0057**	0.0234
						2.2731	2.7574	2.5167	2.7071	2.7450	7.9124	2.6015	1.7535	2.4933	1.9904	2 3972
10						0.0024	0.0173	0.0391	0.2147	0.0731	**0.1438**	**0.0199**	**0.2935**	**0.0008**	**0.1328**	**0.0016**
						2.8540	2.4603	2.8204	2.5827	2.7028	2.7445		2 6355	0.9430	2.5500	1.6629
11						0.0012	0.0017	0.0419	0.0142	0.2877	0.0114	0.0588	0.0159	**0.2822**	**0.0044**	**0.1772**
						2.5095	3.0320	2.5587	2.9357	2.6241	2.6752	2.7342		2.6642		2.6090
12							0.0035	0.0008	0.0740	0.0009	0.2971	0.0014	0.0047	0.0030	0.2168	0.0093
							2.6106	3.7550	2.6263	3.3908	2.6517	2.4623	2.7071		2.6851	
13								0.0069	0.0038	0.0944	0.0276	0 2207	0.0147	0.0115	0.0039	0.1108
								2.6966	1.4144	2.6820	1.8068	2.6692	3.0149	2.6427		2.6957
14								0.0015	0.0082	0.0270	0.0764	0.1026	0.0979	0.0114	0.0518	0.0357
								2.2904	2.7917	2.3237	2.7376	2.4543	2.6761	2.8762	2.4668	
15									0.0066	0.0030	0.0778	0.0225	0.1665	0.0136	0.0010	0.0528
									2.4973	2.9426	2.5114	2.8099	2.5766	2.6662	2.8449	1.6156

Table 3a *(Cont'd.)*

V'/V"	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
0																
1																
2																
3																
4																
5																
6																
7	0.0018															
	2.2414															
8	0.0032	0.0032	0.0011													
	2.1409	2.2678	2.1377													
9	0.0234	**0.0032**	**0.0058**	**0.0015**	**0.0017**											
	2.3972	2.0497	2.3122	2.0866	2.2492											
10	**0.0016**	**0.0392**	**0.0023**	**0.0109**	**0.0017**	**0.0034**	**0.0010**	**0.0012**								
	1.6629	2.4649	1.8570	2.3788	1.9812	2.3013	2.0899	2.2499								
11	**0.1772**	**0.0009**	**0.0658**	**0.0010**	**0.0212**	**0.0013**	**0.0071**	**0.0012**	**0.0026**							
	2.6090		2.5453	1.3513	2.4672	1.7430	2.3768	1.9933	2.2958							
12	0.0093	**0.2116**	0.0042	**0.1049**	**0.0008**	**0.0409**	**0.0010**	**0.0150**	**0.0009**	**0.0057**	**0.0009**	**0.0022**				
		2.6645		2.6297		2.5696	1.0420	2.4752	1.7757	2.3651	2.0464	2.2779				
13	0.1108	0.0053	**0.2062**	0.0113	**0.1481**	**0.0048**	**0.0740**	**0.0009**	**0.0316**	**0.0010**	**0.0127**	**0.0005**	**0.0051**			
	2.6957		2.7123		2.7088		2.6734		2.5884	1.1602	2.4607	1.8770	2.3379			
14	0.0357	0.0213	0.0011	0.1400	0.0102	**0.1670**	**0.0134**	**0.1162**	**0.0061**	**0.0619**	**0.0012**	**0.0285**	**0.0011**	**0.0121**		
		2.6920		2.7495	3.9519	2.7762		2.7672		2.7030		2.5777	1.4319			
15	0.0528	0.0664	0.0016	0.0270	0.0445	0.0010	0.1252	0.0135	0.1392	**0.0166**	**0.1019**	**0.0096**	**0.0584**	**0.0035**	**0.0285**	
	1.6156	1.8815	2.6652		2.7743	3.6549	2.8295	3 6827	2 8447	4 0043	28066		2.7033			

Table 3b. Franck Condon factors and r-centroids for the $B^1\Pi_1 - X^1\Sigma^+$ transition of $^{71}Ga^{127}I$.

v'/v''	0	1	2	3	4	5	6	7	8	9	10
0	**0.9165**	**0.0647**	0.0164	0.0020							
	2.5665	2.3974	2.4366	2.3342							
1	**0.0812**	**0.8000**	**0.0743**	0.0377	0 0050	0.0014					
	2.7098	2.5787	2.3462	2.4523	2.3057	2.3662					
2	**0.0015**	**0.1240**	**0.7427**	0.0583	0.0617	0.0076	0.0034				
	2.2338	2.7253	2.5930	2.2548	2.4754	2.2561	2 3888				
3		**0.0087**	**0.1342**	**0.7159**	0 0340	0.0897	0 0084	0 0066			
		2.3878	2.7440	2.6080	2.0725	2.5055	2.1652	2 4219			
4		0.0023	**0.0273**	**0.1159**	**0.6955**	0.0130	0 1245	0 0070	0.0118	0 0013	0.0011
		2.7979	2.4767	2.7680	2.6200	1 6168	2.5405	1.9815	2.4657	2.1000	2.3946
5			0.0034	**0.0626**	0.0768	**0.6589**	0.0016	0.1679	0.0037	0.0204	0.0013
			2.8937	2.5361	2.8030	2 6337		2.5770	1.5214	2.5173	1.8940
6			0.0015	0.0027	0 1150	0.0320	0.5871	0.0003	0.2192	0.0006	0.0345
			2.5327	3.0964	2 5793	2.8725	2 6405		2.6113		2.5719
7				0.0046	0.0004	0.1750	0.0027	0.4721	0.0050	0.2717	0.0005
				2.6039		2.6123	3.2507	2.6395		2.6403	
8					0 0101	0 0019	0.2223	0.0082	0 3244	0.0067	0.3110
					2.6643	1.7247	2 6374	2.4566	2.6241		2.6614
9						0.0161	0.0187	0 2335	0.0516	0.1769	0.0024
						2.7244	2.3344	2.6551	2.6523	2.5775	
10						0.0035	0.0188	0.0618	0.2027	0.1086	0.0699
						2.4370	2.7961	2.4852	2.6625	2.7063	2.4462

Franck Condon values ≥ 0.001 are only included.

The r-centroid values are below the Franck Condon values.

The bold values of FCF's are the bands observed.

that all the additional bands observed towards lower wave number region, after the reversal of degradation, belongs to the negative sequences of A-X transition.

Acknowledgments

The authors express their sincere thanks to Dr. V P Bellary and Dr. T K Balasubramanian for encouragement and helpful suggestions in the course of this work.

References

[1] M D Saksena, R Venkatasubramanian and M Singh *Can. J. Phys.* **75** 191 (1997)

[2] R Venkatasubramanian, M D Saksena and M Singh *J. Mol. Spectrosc.* **168** 290 (1994)

[3] M D Saksena, K Sunanda and G Lakshminarayana *J. Phys.* **B27** 3735 (1994)

[4] K Sunanda, M D Saksena and G Lakshminarayana *J. Mol. Spectrosc.* **168** 158 (1994)

[5] K P R Nair, H U Schutze-Pahlmann and J Hoeft *Chem. Phys. Lett.* **70** 583 (1980)

[6] E Tiemann, M Grasshoff and J Hoeft *Z. Naturforsch.* **A27** 753 (1972)

[7] W R Jarmain and J C McCallum *J. Quant. Spectrosc. Radiative Transfer* **11** 421 (1971)